AN EXPONENTIAL TIME DIFFERENCING METHOD FOR THE NONLINEAR SCHRÖDINGER EQUATION

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Abstract. The spectral methods offer very high spatial resolution for a wide range of nonlinear wave equations, so, for the best computational efficiency, it should be desirable to use also high order methods in time but without very strict restrictions on the step size by reason of numerical stability. In this paper we study the exponential time differencing fourth-order Runge-Kutta (ETDRK4) method; this scheme was derived by Cox and Matthews in [6] and was modified by Kassam and Trefethen in [14]. We compute its amplification factor and plot its stability region, which gives us an explanation of its good behavior for dissipative and dispersive problems. We apply this method to the Schrödinger equation, obtaining excellent results for the cubic equation and the critical exponent case and, later, as an experimental approach to describe the various possible asymptotic behaviors with two space variables.

1. Introduction

The spectral methods have been shown to be remarkably successful when solving time-dependent partial differential equations (PDEs). The idea is to approximate a solution $u(x, t)$ by a finite sum $v(x, t) = \sum_{k=0}^{N} a_k(t)\phi_k(x)$, where the function class $\phi_k(x), k = 0, 1, \ldots, N$, will be trigonometric for $x$–periodic problems and, otherwise, an orthogonal polynomial of Jacobi type, with Chebyshev polynomial being the most important special case. To determine the expansion coefficients $a_k(t)$, we will focus on the pseudo-spectral methods, where it is required that the coefficients make the residual equal zero at as many (suitably chosen) spatial points as possible. Three books [10], [4] and [23] have been contributed to supplement the classic references [12] and [3].

When a time-dependent PDE is discretized in space with a spectral simulation, the result is a coupled system of ordinary differential equations (ODEs) in time: it is the notion of the method of lines (MOL) and the resulting set of ODEs is stiff; the stiffness problem may be even exacerbated sometimes, for example, using Chebyshev polynomials (see Chapter 10 of [23] and its references). The linear terms are primarily responsible for the stiffness with rapid exponential decay of some modes (as with a dissipative PDE) or a rapid oscillation of some modes (as with a dispersive PDE). Therefore, for a time-dependent PDE which combines low-order nonlinear terms with higher-order linear terms it is desirable to use higher-order approximation in space and time.

The structure of this paper is as follows. In Section 2 we describe the ETDRK4 (Exponential Time Differencing fourth-order Runge-Kutta) method by Cox and
Matthews in [6] and the modification proposed by Kassam and Thefethen in [14]. We discuss the stability of the ETDRK4 method in Section 3. In Sections 4 and 5 we test the method for the nonlinear Schrödinger equation in one and two space dimensions and, finally, we summarize our conclusions.

2. Exponential Time Differencing fourth-order Runge-Kutta Method

The numerical method considered in this paper is an exponential time differencing (ETD) scheme. These methods arose originally in the field of computational electrodynamics [22]. Since then, they have recently received attention in [3] and [19], but the most comprehensive treatment, and in particular the ETD with Runge-Kutta time stepping, is in the paper by Cox and Matthews [6].

The idea of the ETD methods is similar to the method of the integrating factor (see for example [4] or [23]): we multiply both sides of a differential equation by some integrating factor, then we make a change of variable that allows us to solve the linear part exactly and, finally, we use a numerical method of our choice to solve the transformed nonlinear part.

When a time-dependent PDE in the form

\[ u_t = \mathcal{L}u + \mathcal{N}(u, t), \]

where \( \mathcal{L} \) and \( \mathcal{N} \) are the linear and nonlinear operators respectively, is discretized in space with a spectral method, the result is a coupled system of ordinary differential equations (ODEs),

\[ u_t = \mathbf{L}u + \mathbf{N}(u, t). \]

Multiplying (2.2) by the term \( e^{-\mathcal{L}t} \), known as the integrating factor, gives

\[ e^{-\mathcal{L}t}u_t - e^{-\mathcal{L}t}\mathcal{L}u = e^{-\mathcal{L}t}\mathcal{N}(u, t), \]

and with the new variable \( v = e^{-\mathcal{L}t}u \), we find the transformed equation

\[ v_t = e^{-\mathcal{L}t}\mathcal{N}(e^{\mathcal{L}t}v, t), \]

where the linear term is gone; now we can use a time stepping method of our choice to advance in time. However, the integrating factor methods can also be a trap, for example, to model the formation and dynamics of solitary waves of the KdV equation (see Chapter 14 of [4]). A second drawback is the large error constant.

In the derivation of the ETD methods, following [3], instead of changing the variable, we integrate (2.3) over a single time step of length \( h \), getting

\[ u_{n+1} = e^{\mathcal{L}h}u_n + e^{\mathcal{L}h} \int_0^h e^{-\mathcal{L}\tau}\mathcal{N}(u(t_n + \tau), t_n + \tau) d\tau. \]

The various ETD methods come from how one approximates the integral in this expression.

Cox and Matthews derived in [6] a set of ETD methods based on the Runge-Kutta time stepping, which they called ETDRK methods. In this paper we consider
the ETDRK4 fourth-order scheme with the formulae

\begin{align*}
a_n &= e^{Lh/2}u_n + L^{-1}(e^{Lh/2} - 1)N(u_n, t_n), \\
b_n &= e^{Lh/2}u_n + L^{-1}(e^{Lh/2} - 1)N(a_n, t_n + h/2), \\
c_n &= e^{Lh/2}a_n + L^{-1}(e^{Lh/2} - 1)(2N(b_n, t_n + h/2) - N(u_n, t_n)), \\
u_{n+1} &= e^{Lh}u_n + h^{-2}L^{-3}\left\{-4I - hL + e^{Lh}(4I - 3hL + (hL)^2)\right\}N(u_n, t_n) \\
&\quad + 2[2I + hL + e^{Lh}(-2I + hL)](N(a_n, t_n + h/2) + N(b_n, t_n + h/2)) \\
&\quad + [-4I - 3hL - (hL)^2 + e^{Lh}(4I - hL)]N(c_n, t_n + h).
\end{align*}

More detailed derivations of the ETD schemes can be found in [6].

Unfortunately, in this form ETDRK4 suffers from numerical instability when \( L \) has eigenvalues close to zero, because disastrous cancellation errors arise. Kassam and Trefethen have studied in [14] these instabilities and have found that they can be removed by evaluating a certain integral on a contour that is separated from zero. The procedure is basically to change the evaluation of the coefficients, which is mathematically equivalent to the original ETDRK4 scheme of [6], but in [9] it has been shown to have the effect of improving the stability of integration in time. Also, it can be easily implemented and the impact on the total computing time is small. In fact, we have always used this idea in our \textit{MATLAB}⃝ codes.

3. ON THE STABILITY OF ETDRK4 METHOD

The stability analysis of the ETDRK4 method is as follows (see [9], [11] or [6]). For the nonlinear ODE

\begin{equation}
\frac{du}{dt} = cu + F(u),
\end{equation}

with \( F(u) \) the nonlinear part, we suppose that there exists a fixed point \( u_0 \); this means that \( cu_0 + F(u_0) = 0 \). Linearizing about this fixed point, if \( u \) is the perturbation of \( u_0 \) and \( \lambda = F'(u_0) \), then

\begin{equation}
u_t = cu + \lambda u
\end{equation}

and the fixed point \( u_0 \) is stable if \( \text{Re}(c + \lambda) < 0 \).

The application of the ETDRK4 method to (3.2) leads to a recurrence relation involving \( u_n \) and \( u_{n+1} \). Introducing the previous notation \( x = \lambda h, \ y = ch \) and using the \textit{Mathematica}⃝ algebra package, we obtain the following amplification factor

\begin{equation}
\frac{u_{n+1}}{u_n} = r(x, y) = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + c_4 x^4,
\end{equation}

where
\[c_0 = e^y,\]
\[c_1 = \frac{-4}{y^3} + \frac{8e^y}{y^5} - \frac{8e^{3y}}{y^3} + \frac{4e^{2y}}{y^3} - \frac{1}{y^2} + \frac{4e^y}{y^2} - \frac{6e^y}{y^2} + \frac{4e^{3y}}{y^2} - \frac{e^{2y}}{y^2},\]
\[c_2 = \frac{-8}{y^3} + \frac{16e^y}{y^5} - \frac{16e^{3y}}{y^3} + \frac{8e^{2y}}{y^3} - \frac{5}{y^2} + \frac{12e^y}{y^2} - \frac{10e^y}{y^2} + \frac{4e^{3y}}{y^2} - \frac{e^{2y}}{y^2},\]
\[c_3 = \frac{4}{y^3} + \frac{16e^y}{y^5} + \frac{16e^{3y}}{y^3} - \frac{20e^{2y}}{y^3} + \frac{8e^{3y}}{y^3} + \frac{2}{y^2} + \frac{10e^y}{y^2} + \frac{16e^y}{y^2} - \frac{12e^{3y}}{y^2} + \frac{6e^{2y}}{y^2} - \frac{2e^y}{y^2} + \frac{2e^{3y}}{y^2} - \frac{2e^{2y}}{y^2},\]
\[c_4 = \frac{8}{y^6} - \frac{24e^y}{y^6} + \frac{16e^y}{y^5} + \frac{16e^{3y}}{y^5} - \frac{24e^{2y}}{y^5} + \frac{8e^{3y}}{y^5} + \frac{6}{y^4} - \frac{18e^y}{y^4} + \frac{20e^y}{y^4} - \frac{12e^{3y}}{y^4} + \frac{6e^{2y}}{y^4} - \frac{2e^y}{y^4} + \frac{2e^{3y}}{y^4} - \frac{6e^y}{y^4} - \frac{2e^{3y}}{y^4}.\]

An important remark: computing \(c_1, c_2, c_3\), and \(c_4\) by the above expressions suffers from numerical instability for \(y\) close to zero. Because of that, for small \(y\), instead of them, we will use their asymptotic expansions

\[c_1 = 1 + y + \frac{1}{2}y^2 + \frac{1}{6}y^3 + \frac{13}{320}y^4 + \frac{7}{960}y^5 + \mathcal{O}(y^6),\]
\[c_2 = \frac{1}{2} + \frac{1}{2}y + \frac{1}{4}y^2 + \frac{1}{4}y^3 + \frac{247}{2880}y^4 + \frac{131}{5760}y^5 + \frac{479}{96768}y^6 + \mathcal{O}(y^6),\]
\[c_3 = \frac{1}{6} + \frac{1}{6}y + \frac{1}{2}y^2 + \frac{1}{36}y^3 + \frac{1441}{241920}y^4 + \frac{441}{120960}y^5 + \mathcal{O}(y^6),\]
\[c_4 = \frac{1}{24} + \frac{1}{32}y + \frac{7}{640}y^2 + \frac{19}{11520}y^3 - \frac{25}{64512}y^4 - \frac{311}{860160}y^5 + \mathcal{O}(y^6).\]

We make two observations:

- As \(y \to 0\), our approximation becomes
  \[r(x) = 1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 + \frac{1}{24}x^4;\]
  which is the stability function for all the 4-stage Runge-Kutta methods of order four.
- Because \(c\) and \(\lambda\) may be complex, the stability region of the ETDRK4 method is four-dimensional and therefore quite difficult to represent. Unfortunately, we do not know any expression for \(|r(x, y)| = 1\); we will only be able to plot it.

The most common idea is to study it for each particular case; for example, assuming \(c\) to be fixed and real in \([3]\) or that both \(c\) and \(\lambda\) are pure imaginary numbers in \([11]\). We provide several examples of stability regions in situations that interest us.
For dissipative PDEs with periodic boundary conditions, the scalars $c$ that arise with a Fourier spectral method are negative. Let us take for example Burger's equation

\begin{equation}
\frac{\partial u}{\partial t} = \epsilon \frac{\partial^2 u}{\partial x^2} - \left( \frac{1}{2} u^2 \right)_{x}, \quad x \in [-\pi, \pi],
\end{equation}

with $0 < \epsilon \ll 1$. Transforming it to the Fourier space gives

\begin{equation}
\hat{u}_t = -\epsilon \xi^2 \hat{u} - \frac{i \xi}{2} \hat{u}^2, \quad \forall \xi,
\end{equation}

where $\xi$ is the Fourier wave-number and the coefficients $c = -\epsilon \xi^2 < 0$ span over a wide range of values when all the Fourier modes are considered. For high values of $|\xi|$, the solutions are attracted to the slow manifold quickly because $c < 0$ and $|c| \ll 1$.

In Figure 1 we draw the boundary stability regions in the complex plane $x$, for $y = 0, -0.9, -5, -10, -18$, which are similar to Figures 3.2, 3.3 and 3.4 of [9]. When the linear part is zero ($y = 0$), we recognized the stability region of the fourth-order Runge-Kutta methods and, as $y \to -\infty$, the region grows. Of course, these regions only give an indication of the stability of the method.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{stabilityregions.png}
\caption{Boundary of stability regions for several negative $y$}
\end{figure}

In fact, for $y < 0, |y| \ll 1$ the boundaries that are observed approach to ellipses whose parameters have been fitted numerically with the following result

\begin{equation}
(Re(x))^2 + \left( \frac{Im(x)}{0.7} \right)^2 = y^2.
\end{equation}
In Figure 2 we draw the experimental boundaries and the ellipses (3.6) with $y = -75$.

![Figure 2. Experimental boundaries and ellipse for $y = -75$](image)

Figure 2. Experimental boundaries and ellipse for $y = -75$

The spectrum of the linear operator increases as $\xi^2$, while the eigenvalues of the linearization of the nonlinear part lay on the imaginary axis and increase as $\xi$. On the other hand, according to (3.6), when $Re(x) = 0$, the intersection with the imaginary axis $Im(x)$ increases as $|y|$, i.e., as $\xi^2$. Since the boundary of stability grows faster than $x$, the ETDRK4 method should have a very good behavior to solve Burger’s equation, which confirms the results of paper [14]. A similar analysis is applicable to other dissipative equations like, for instance, the Kuramoto-Sivashinsky equation or the Allen-Cahn equation of [6] or [14], where $h = 1/4$.

4. **Nonlinear Schrödinger Equation in One Space Variable**

The nonlinear Schrödinger equation arises in a number of situations in which the envelope solutions of weakly nonlinear dispersive systems are described. The one-dimensional case is

\begin{align}
\begin{align*}
    iu_t + u_{xx} + q|u|^p u &= 0, & (x, t) \in (-\infty, \infty) \times (0, T], \\
    u(x, 0) &= u_0(x), & x \in (-\infty, \infty),
\end{align*}
\end{align}

(4.1) (4.2)

where $q$ and $p$ are real constants with $p > 0$ and the sign of $q$ gives two very different problems: the focusing case if $q > 0$ and the defocusing one for $q < 0$. The initial conditions include the case where $|u_0(x)| \to 0$ as $|x| \to \infty$, which we call the infinite line problem, and also the periodic case where $u_0(x + L) = u_0(x)$.
The solution of (4.1) satisfies at least two conservation laws: the $L^2$ norm
\[ C = \|u(\cdot, t)\|_2, \quad \forall t \in \mathbb{R}, \]
and
\[ H = \|u_x(\cdot, t)\|_2^2 - \frac{2q}{p + 2} \|u(\cdot, t)\|_{p + 2}^{p + 2}, \quad \forall t \in \mathbb{R}. \]

Moreover, this equation has travelling wave solutions of the form
\[ u(x, t) = f(x - ct, \beta) \exp\left( \frac{icx - bt}{2} \right), \]
which travel with speed $c$; $b$ is an arbitrary parameter, $\beta = c^2 (\frac{c^2}{2} - b)$ and
\[ f(x, \beta) = \left( \frac{p + 2}{2q} \right) \left( \frac{p}{2} \sqrt{\beta x} \right)^{1/p}. \]

When the spatial part is discretized using a Fourier spectral method, transforming it to the Fourier space gives
\[ \hat{u}_t = -i\xi^2 \hat{u} + iq \langle u^p u \rangle, \quad \forall \xi; \]
therefore, the eigenvalue of the linear operator is pure imaginary and the stability regions are quite different. In Figures 3 and 4 we draw from top to bottom and left to right the boundary stability regions for $y = -10i$, $y = 10i$ and $y = -75i$, $y = 75i$ respectively. It must be understood that these regions only give an indication of the stability of the method. We observe that the stability regions include an interval of the imaginary axis, till exactly the value $-y$. Again, using Mathematica, we have checked that
\[ |r(\beta i, -\beta i)| = 1, \quad \forall \beta. \]
This argument gives an indication of the stability of the ETDRK4 method applied to the equation (4.1), with the excellent results that we expose next.

![Figure 3. Boundary of stability regions for $y = -10i$ and $y = 10i$](image)

The experiments were carried out in our 1.60 Ghz Fujitsu Siemens laptop. The time step is 0.01 and 0.001 and the maximum computer time is about 30 or 40 seconds.

We would like to point out that we do not try to preserve any invariants of the equation or any phase space properties, neither to compare this method with others as it has already been made in [13], [15], [1] and [2], all of them having coincided in the clear superiority of ETDRK4 in front of the other methods from the point
of view of both efficiency and speed. We will rather try to reproduce with the ETDRK4 method the theoretical results gathered from reference [17].

First, we consider $p = 2$, the so-called cubic nonlinear Schrödinger equation. In this case, the travelling waves (4.3) are solitons because they retain their shape even after interaction among themselves, i.e., they act somewhat like particles; see, for example, [16] or [8]. The initial condition used is

$$g(x) = \frac{\sqrt{2\beta}}{q} \text{sech}(\sqrt{\beta}x).$$

This function is not mathematically periodic, but it can be regarded as being periodic in practice because it is very close to zero at the ends of the interval.

To study the interaction of two solitons, we assume that the initial condition is the superposition of the solitons with different speeds. In Figure 5 on the left, we can check how our method reproduces the elastic collision of both solitons with the very well-known landslide in phase.

$$u_0(x) = \text{sech}(x),$$
which, according to (4.7), gives rise to a stationary soliton provided that $q = 2$, but complex phenomena may be originated for other values of $q$. For $q = 2Q^2$, $Q = 2, 3, \ldots$, Miles has shown in [18] that (4.8) will evolve into a bound state of $Q$ solitons, all moving at the same speed. In Figure 5 on the right for $q = 8$ and in Figure 6 for the cases $q = 18, 32$, we plot the modulus of the numerical solutions with initial condition $\text{sech}(x)$. For $q = 8$ the graph reaches a spike, followed by a low area and a second spike and, then, it returns to its initial shape to begin another period. For $q = 18$ the graph reaches a spike, followed by a pair of symmetric ridges, followed by a second spike; finally, for $q = 32$ we can observe three ridges between two spikes.

**Figure 6.** Cubic Schrödinger equation with $q = 18$ and $q = 32$

As a final test, we have checked the behavior of our method for the problem of the critical exponent $p = 4$; this means that the asymptotic behavior of the solutions of (4.1) is very different. Theorem 6.2 at page 124 of [17] proves the extension globally in time of the local solutions under any of the following hypotheses:

- **Defocusing case**: $q < 0$. In Figure 7 we can appreciate the typical dispersion.
- **Focusing case**: $q > 0$ and $\|u_0\|_2 \leq c_0$. Moreover, Weinstein in [24] estimates the value of the constant $c_0 = \|\psi\|_2$, where $\psi$ is a positive solution of the equation $\psi'' - \psi + \psi^5 = 0$ of minimal $L^2$ norm, i.e.,

\[
(4.9) \quad \psi(x) = \sqrt{\frac{3}{4} \sqrt{\text{sech}(x)}} \approx 0.9306 \sqrt{\text{sech}(x)}.
\]

In Figure 8 we can check the numerical solutions with the initial condition $\psi(x)$ on the left and with the initial condition $0.94 \sqrt{\text{sech}(x)}$ on the right with a blow-up in finite time.

5. The two-dimensional nonlinear Schrödinger equation

Bearing in mind the good behavior of our simulation for the one-dimensional problem and the fact that MATLAB also implements higher dimensional discrete Fourier transforms and their inverses (in two variables, we have `fft2` and `ifft2`), we thought that small modifications of our program would allow us to simulate the two-dimensional cubic nonlinear Schrödinger equation.
Figure 7. Defocusing case: \( p = 4 \) and \( q = -1 \)

Figure 8. Focusing case: \( p = 4 \) and \( q = 1 \)

\[(5.1) \quad iu_t + u_{xx} + u_{yy} + q|u|^2 u = 0, \quad (x, y) \in \mathbb{R}^2, t > 0.\]

This mathematical model occurs in many physical applications; it is especially relevant in Optics (more details in [21]). This equation has been intensively studied but its behaviors are not understood completely (see [21], [20], [13] and their references for details).

A very important question concerns the conditions of stability or instability of the standing wave solutions. It is well known that for \( q > 0 \) (focusing case), the larger wave numbers are stabilized by dispersion, while the smaller ones are linearly unstable. This case is also the one studied in [24] and, when \( \|u_0\|_2 \) is above a threshold value, the solution of (5.1) can self-focus and become singular in finite time; this phenomenon is called wave collapse or blow-up of the wave amplitude.

In our first test with \( q = 1 \) and the initial condition

\[(5.2) \quad u_0(x, y) = 2 + 0.01 \sin(x + \frac{\pi}{4}) \sin(y + \frac{\pi}{4}), \quad (x, y) \in [-\pi, \pi] \times [-\pi, \pi],\]

with \( \|u_0\|_2 \approx 12.56 \), using \((256)^2\) collocations points, we have obtained Figure 9 which reproduces Figure 1.1 of [21]. The computer time takes about 64.30 seconds.
In the second test we try to observe the differences between \( q = 1 \) and \( q = -1 \) and the blow-up case with the initial condition

\[
(5.3) \quad u_0(x, y) = \alpha \cdot \text{sech}(x^2 + y^2), \quad (x, y) \in [-20, 20] \times [-20, 20],
\]

where \( \alpha \) is a real parameter; now, \( \|u_0\|_2 = \alpha \sqrt{\pi} \).

In Figure 10, we have drawn the evolution in time for \( \alpha = 5, q = 1 \), with \( \|u_0\|_2 \approx 8.8623 \). We can observe that the dispersion process dominates. On the contrary, for the case \( q = -1 \) shown in Figure 11, the dominating process is the dissipative one.

Finally, in Figure 12 we have represented the evolution with \( \alpha = 6 \); in that case, \( \|u_0\|_2 \approx 10.6347 \). The computed blow-up happens quite fast, at \( t = 0.1 \); the height of the solution is about 11.89 and for \( t = 0.11 \), it is 259.90.

6. Conclusions

The proposers of the ETDRK schemes in [6] concluded that they are more accurate than other methods (standard integrating factor techniques or linearly implicit schemes); they have good stability properties and are widely applicable to nonlinear wave equations. However, Cox and Matthews were aware of the numerical instability for the ETDRK4 method when computing the coefficients. Later, Kassan and Trefethen in [14] modified the ETDRK4 method with very good results. In the opinion of these authors, the modified ETDRK4 is the best by a clear margin compared with others methods.

We have computed and studied the numerical stability function of the ETDRK4 methods and, besides their good stability properties, we have exposed the reasons of their good behavior for dissipative and dispersive problems.
In addition, we have applied this method to the Schrödinger equations (4.1) and (5.1), achieving the excellent results that we have just mentioned. It would be interesting to implement this method for non-periodic boundary condition problems in two dimensions, for which another kind of orthogonal polynomials would be
Figure 12. Initial condition (5.3) with $\alpha = 6 \ q = 1$ required (Chebyshev, Hermite...), and to simulate numerically the results obtained by [13].

We think that even the incompressible Navier-Stokes equations could be simulated with the proposed method (see, for example [3]). Recently, in [7], we simulated the blow-up of semi-linear diffusion equations in one and two spatial dimensions with very good results.

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